WHAT IS CLAIMED IS:

**What is claimed is:**

1.      A method for generating atomic coordinates from a set of interatomic distance and/or volume constraints, the method comprising the steps of:

(1)     placing a set of atoms on a coordinate map;

(2)     selecting a subset of atoms from the set of atoms, wherein the subset of atoms includes at least one associated constraint between the atoms in the subset;

(3)     revising at least one coordinate of at least one atom from the selected subset of atoms on the coordinate map based on the at least one associated constraint when the at least one associated constraint is violated;

(4)     repeating steps (2) and (3) for additional subsets of atoms from the set of atoms; and

(5)     generating coordinates for the set of atoms.

2.      The method of claim (1), wherein the set of constraints includes a set of distance constraints.

3.      The method of claim (1), wherein the set of constraints includes a set of volume constraints.

4.      The method of claim (2), wherein the subset of atoms includes two atoms.

5.      The method of claim (3), wherein the subset of atoms includes four atoms.

6.      The method of claim (1), wherein the set of atoms includes at least one real atom.

7.      The method of claim (1), wherein the set of atoms includes at least one abstracted atom.

8.      The method of claim (1), wherein the subset of atoms is chosen at random.

9.     The method of claim (1), wherein the subset of atoms is chosen with a probability that depends on whether the at least one associated constraint is a distance constraint or a volume constraint.

10.    The method according to claim (1), wherein step (3) comprises the step of adjusting at least one coordinate of at least one atom from the selected subset of atoms on the coordinate map by a correction factor so that the degree of violation of at least one associated constraint is improved upon adjusting the at least one coordinate.

11.    The method according to claim (10), further comprising the steps of repeating steps (2) through (4) for several correction factors.

12.    The method of claim (1), further comprising the step of:

     (6)     generating the distance and volume constraints from connectivity and covalent bond lengths and angles associated with the selected set of atoms.